

# Site-Specific Valence Band Photoemission from the Perovskite $\text{La}_{1/2}\text{Sr}_{3/2}\text{MnO}_4$ Using X-Ray Standing Waves

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Beamline(s): **X24A**

By creating an X-ray standing wavefield around a bulk Bragg reflection, we can maximize the X-ray field intensity at different positions within the unit cell of the perovskite  $\text{La}_{1/2}\text{Sr}_{3/2}\text{MnO}_4$ . From the observed differences in the valence band photoemission spectra as the wavefield position is moved, one can determine experimentally the contributions of valence electrons in different parts of the unit cell to energy states in the  $\text{La}_{1/2}\text{Sr}_{3/2}\text{MnO}_4$  valence band.

The perovskite structure is common to colossal magnetoresistive (manganite) and high- $T_C$  superconducting (cuprate) materials. The origin of these effects are the Mn-O (or Cu-O) planes in the layered planar tetragonal structure of the perovskites, and "charge ordering" and "orbital ordering" of valence electrons in the Mn-O plane have been seen at low temperatures (below  $T_{CO} = 217$  K for  $\text{La}_{1/2}\text{Sr}_{3/2}\text{MnO}_4$ ).

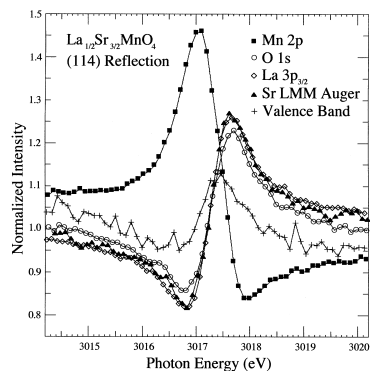
Experiments were performed at beamline X24A at the NSLS. The  $\text{La}_{1/2}\text{Sr}_{3/2}\text{MnO}_4$  sample was cleaved in ultrahigh vacuum ( $10^{-10}$  torr) to expose the (001) surface. Four reflections – (114), (116), (204), and (213) – were examined in the backreflection configuration, at Bragg energies of  $h\nu = 3017.3$  eV, 3750.1 eV, 3773.8 eV, and 3882.6 eV, respectively. The increased angular width of Bragg reflections in backreflection accommodates the mosaicity of the sample. The monochromator crystals were Si(111).

Figure 1 shows the (114) photoemission XSW yields, respectively, of La, Mn, and O core-levels, and the Sr LMM Auger XSW yield, as well as the valence band photoemission XSW yield, taken with a hemispherical analyzer energy window which surrounds the entire valence band. The O 1s and La  $3p_{3/2}$  core-level yields and Sr LMM Auger yield as well as the valence emission yield have a lineshape corresponding to a coherent position of zero, while the Mn 2p yield corresponds to a coherent position of 1/2. The valence band emission has a coherent fraction near zero, and looks more like the reflectivity. This lineshape suggests the contributions from Mn (coherent position 1/2) to the valence emission are similar in magnitude to the combined contributions from La, Sr, and O (coherent position 0), so the total X-ray structure factor for valence band emission cancels out.

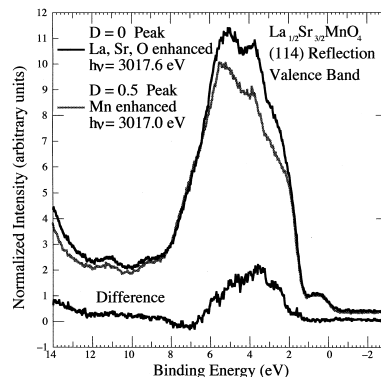
By setting the photon energy at the values for the maximum of the core-level XSW yields for either coherent position 0 or 1/2, we increase the X-ray electric field intensity and therefore electron emission at this position, while emission is minimized at the opposite position. Figure 2 shows high-resolution photoemission spectra taken at these two photon energies, as well as a difference spectrum. Emission at the higher binding energy part of the valence band is enhanced when the standing wavefield is maximized on the Mn positions, indicating a higher density of Mn valence states at these energies. Similarly, the lower binding energy part of the valence band is higher in La, Sr, and O valence state density.

The results for (204) reflection, which also separates Mn atoms from La, Sr, and O atoms in terms of coherent position, are similar to the (114) reflection data shown. However, the (116) and (213) reflections, which separate the O atoms in the Mn-O planes from those outside them, show no change in the valence band spectra lineshape as one moves the standing wavefield. This suggests that O 2p emission is very weak within the valence band near 4 keV photon energy, as also has been seen in our experiments on NiO.

References: J.C. Woicik et al., Phys. Rev. Lett. **84**, 773 (2000).



**Figure 1.** Mn 2p, O 1s, La  $3p_{3/2}$ , and core-level photoemission XSW yields, Sr LMM Auger XSW yield and valence band photoemission XSW yield as a function of photon energy for the (114) backreflection of  $\text{La}_{1/2}\text{Sr}_{3/2}\text{MnO}_4$ .



**Figure 2.** High-resolution photoemission spectrum of the  $\text{La}_{1/2}\text{Sr}_{3/2}\text{MnO}_4$  valence band, taken at photon energies at the maximum of the Mn core-level XSW yield ( $h\nu = 3017.0$  eV, shaded line) and at the maximum of the La, Sr, and O core-level XSW yields ( $h\nu = 3017.6$  eV, solid line) for the (114) reflection. Also shown is the difference spectrum.